

UORSY Saturated Fragments Library

Structural motifs with high content of sp^3 -hybridized carbon atoms are widespread in clinically evaluated compounds.¹ Indeed, increasing mean F_{sp^3} of screening collections, called “escape from flatland,”² has been a way to positively influence ADMET profiles. Following the notion, we created a library of saturated fragments. The library contains compounds that comply with “Rule of Three” and have favorable physicochemical profiles (Figure 1, left). Similarity analysis revealed high dissimilarity to the commercially available fragment sets (Figure 1, right).

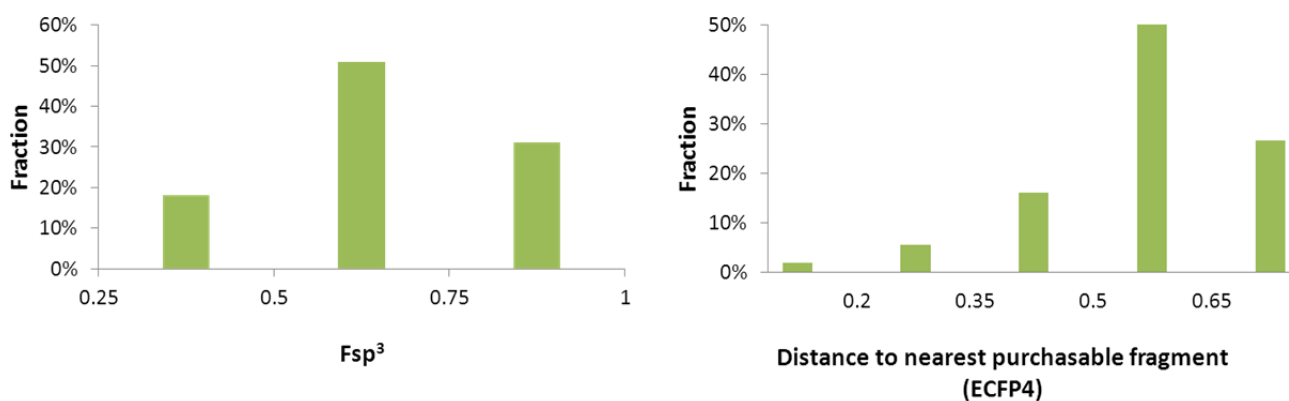
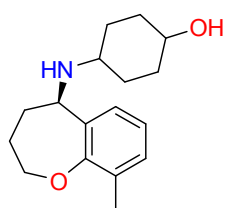
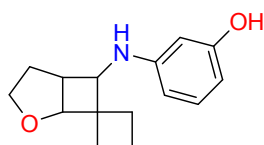


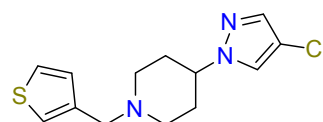
Figure 1. Distribution of F_{sp^3} (left) and similarity analysis (right) of **C saturated fragments**.



PB1436915828



PB1799337364



PB1631773746

Physicochemical profiles of **UORSY saturated fragments**:

$100 < MW < 300$; $HbA \leq 3$; $HbD \leq 3$; $\log P \leq 3$; $RotBonds \leq 3$; $ChiralCenters \leq 4$.

UORSY saturated fragments are available in stock and could be delivered within 2 weeks in any customer-preferred format: as powders, dry films or DMSO solutions formatted in vials, 96 or 384-well plates. All compounds have a minimum purity of 90% assessed by 1H NMR; analytical data is provided.

For more information, please contact us at screenlibs@uorsy.com

¹Morley et al, *Drug Discovery Today*, **2013**, *18*, 1221–1227

²Lovering et al, *J. Med. Chem.* **2009**, *52*, 6752–6756